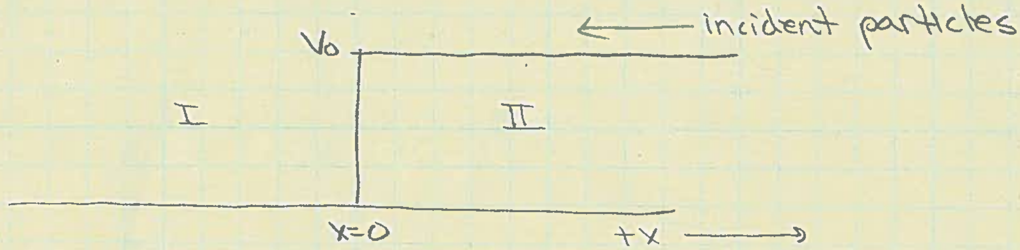
2.33



$E > V_0$

(a) in region I: $\dfrac{d^2\psi}{dx^2} + \dfrac{2m}{\hbar^2} E\psi = 0$

$$k_1^2 = \frac{2m}{\hbar^2}$$

$$\boxed{\psi_1(x) = B_1 e^{-jk_1 x}}$$

* note: there is no component of ψ_1 in the $+x$ direction since region I is semi-infinite

in region II: $\dfrac{d^2\psi}{dx^2} + \dfrac{2m}{\hbar^2}(E - V_0)\psi = 0$

$$k_2^2 = \frac{2m}{\hbar^2}(E - V_0)$$

$$\boxed{\psi_2(x) = A_2 e^{jk_2 x} + B_2 e^{-jk_2 x}}$$

(b) Apply boundary conditions

$\psi_1(0) = \psi_2(0)$ $\qquad\qquad$ $\psi_1'(0) = \psi_2'(0)$

$B_1 = A_2 + B_2$ $\qquad\qquad$ $-jk_1 B_1 = jk_2 A_2 - jk_2 B_2$

$\boxed{B_1 = A_2 + B_2}$ (1) $\qquad\qquad$ $\boxed{k_1 B_1 = k_2 B_2 - k_2 A_2}$ (2)

$R = \dfrac{A_2 \cdot A_2^*}{B_2 \cdot B_2^*} \implies$ need A_2 in terms of B_2

since $k_i = k_r$

$B_1 = A_2 + B_2$ from (1)

plug into (2) $k_1(A_2+B_2) = k_2 B_2 - k_2 A_2$

$$k_1 A_2 + k_1 B_2 = k_2 B_2 - k_2 A_2$$

$$(k_1 + k_2) A_2 = (k_2 - k_1) B_2$$

so $A_2 = B_2 \cdot \dfrac{(k_2-k_1)}{(k_2+k_1)}$

$$\Longrightarrow \boxed{R = \frac{(k_2-k_1)^2}{(k_2+k_1)^2}}$$

$$R+T=1 \Longrightarrow T = 1-R = 1 - \frac{(k_2-k_1)^2}{(k_2+k_1)^2}$$

$$= \frac{(k_2+k_1)^2 - (k_2-k_1)^2}{(k_2+k_1)^2}$$

$$= \frac{\cancel{k_2^2} + 2k_1k_2 + \cancel{k_1^2} - \cancel{k_2^2} + 2k_1k_2 - \cancel{k_1^2}}{(k_2+k_1)^2}$$

$$\boxed{T = \frac{4k_1k_2}{(k_2+k_1)^2}}$$

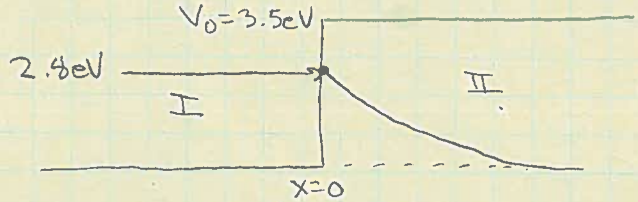
* note: if you 1st calculate T, you must use

$$T = \frac{B_1 \cdot B_1^*}{B_2 \cdot B_2^*} \cdot \frac{v_1}{v_2} = \frac{B_1 \cdot B_1^*}{B_2 \cdot B_2^*} \cdot \frac{k_1}{k_2}$$

since the k-vectors are different on the two sides

2.34

Consider electron with KE = 2.8eV



What is the relative probability of finding the electron at (a) 5Å, (b) 15Å, and (c) 40Å beyond the barrier compared to finding it at the barrier edge

in region II: $\psi(x) = Ae^{-k_2 x}$

$$k_2 = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)} =$$

$$\psi(d) = Ae^{-k_2 d}$$

$$\psi(0) = A$$

so relative probability is $P = \frac{A^2 e^{-2k_2 d}}{A^2} = e^{-2k_2 d}$

see Ex 2.4

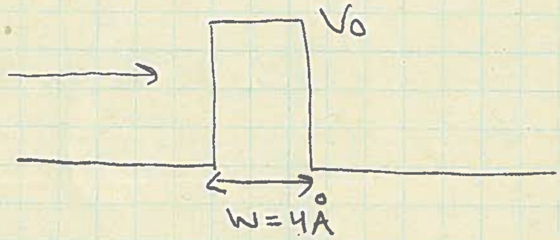
$$k_2 = \sqrt{\frac{2(9.11\times10^{-31}\,kg)(3.5-2.8\,eV)(1.6\times10^{-19}\,J/eV)}{(1.054\times10^{-34}\,J.s)^2}} = 4.29\times10^{9}\,m^{-1}$$

(a) $\exp(-2(4.29\times10^{9}\,m^{-1})(5\times10^{-10}\,m)) = \boxed{0.0137}$

(b) $\exp(-2(4.29\times10^{9}\,m^{-1})(15\times10^{-10}\,m)) = \boxed{2.57\times10^{-6}}$

(c) $\exp(-2(4.29\times10^{9}\,m^{-1})(40\times10^{-10}\,m)) = \boxed{1.24\times10^{-15}}$

$\boxed{2.35}$ $KE = 0.1\,eV$ $V_0 = 1.0\,eV$



$$T = 16\left(\frac{E}{V_0}\right)\left(1-\frac{E}{V_0}\right)\exp(-2k_2 a)$$

(a) $$k_2 = \sqrt{\frac{2(9.11\times10^{-31}\,kg)}{(1.054\times10^{-34}\,J\cdot s)^2}(1.0\,eV - 0.1\,eV)(1.6\times10^{-19}\,J/eV)}$$

$$= 4.86\times10^{9}\,m^{-1}$$

$$T = 16\left(\frac{0.1}{1.0}\right)\left(1-\frac{0.1}{1.0}\right)\exp\left(-2(4.86\times10^{9}\,m^{-1})(4\times10^{-10}\,m)\right)$$

$$= 1.44\cdot 0.0205 \;\boxed{= 0.0295}$$

(b) $$T = 1.44\exp\left(-2(4.86\times10^{9}\,m^{-1})(12\times10^{-10}\,m)\right)\boxed{= 1.24\times10^{-5}}$$

(c) $$J = 1.2\,mA/cm^2 = 1.2\times10^{-3}\,C/cm^2\cdot s$$

$$J_T = \text{charge}\cdot T\cdot\text{incident Flux}$$

$$J_T = q\cdot T\cdot v_i\cdot N$$

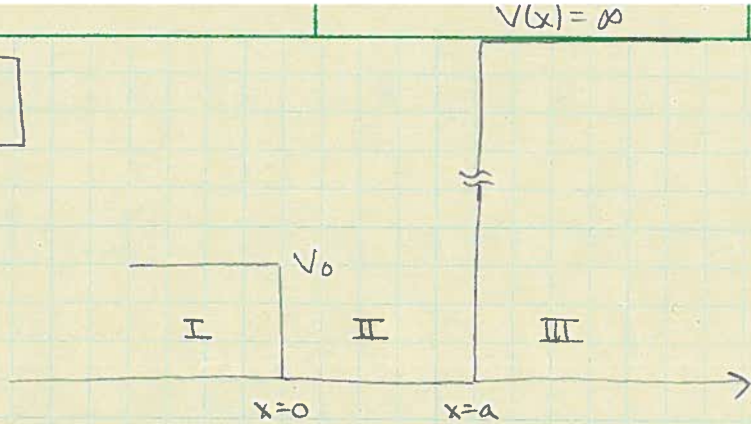
$$E_i = \tfrac{1}{2}mv_i^2 \Rightarrow v_i = \sqrt{\frac{2E}{m}} = \sqrt{\frac{2(0.1\,eV)(1.6\times10^{-19}\,J/eV)}{9.11\times10^{-31}\,kg}}$$

$$= 1.87\times10^{5}\,m/s = 1.87\times10^{7}\,cm/s$$

so $$N = \frac{J_T}{q\cdot T\cdot v_i} = \frac{1.2\times10^{-3}\,\cancel{C}/cm^2\cdot\cancel{s}}{(1.6\times10^{-19}\,\cancel{C})(0.0295)(1.87\times10^{7}\,cm/\cancel{s})}$$

$$\boxed{= 1.36\times10^{10}\,cm^{-3}}$$

2.40



- assume $E < V_0$

(a) write wave solutions in each region

TISE gives: $\dfrac{d^2\psi}{dx^2} + \dfrac{2m}{\hbar^2}(E - V(x))\psi = 0$

region I: $E < V_0$

so $\dfrac{d^2\psi_1}{dx^2} - \dfrac{2m}{\hbar^2}(V_0 - E)\psi_1 = 0$

$\Longrightarrow k_1 = \sqrt{\dfrac{2m(V_0-E)}{\hbar^2}}$

so $\dfrac{d^2\psi_1}{dx^2} - k_1^2\psi_1 = 0$

$\Longrightarrow \psi_1(x) = A_1 e^{k_1 x} + B_1 e^{-k_1 x}$

but $B_1 = 0$ to remain bounded as $x \to -\infty$

so $\boxed{\psi_1(x) = A_1 e^{k_1 x}}$

region II: $V(x) = 0$

so $\dfrac{d^2\psi_2}{dx^2} + \dfrac{2mE}{\hbar^2}\psi_2 = 0$ with $k_2 = \sqrt{\dfrac{2mE}{\hbar^2}}$

so $\boxed{\psi_2(x) = A_2 e^{jk_2 x} + B_2 e^{-jk_2 x}}$ general solution in II

- since $\psi_2(x)$ is "bound" by the well, it is better to use sine and cosine form

$$\boxed{\psi_2(x) = A_2 \cos k_2 x + B_2 \sin k_2 x}$$

in region III: $V(x) = \infty \implies \psi_2(a) = \psi_3(a) = 0$

↳ wave function does not penetrate into region III

- applying the boundary conditions at $x=0$ and $x=a$

$$\psi_1(0) = \psi_2(0) \implies \boxed{A_1 = A_2} \quad (1)$$

$$\psi_2(a) = \psi_3(a) = 0 \implies A_2 \cos k_2 a + B_2 \sin k_2 a = 0$$

$$\implies A_2 \cos k_2 a = B_2 \sin k_2 a$$

$$\implies \boxed{A_2 = -B_2 \tan k_2 a} \quad (2)$$

$$\psi_1'(0) = \psi_2'(0) \implies A_1 k_1 = -A_2 k_2 \sin 0 + B_2 k_2 \cos 0$$

$$\implies \boxed{A_1 = \frac{k_2}{k_1} B_2}$$

$$\implies \boxed{B_2 = \frac{k_1}{k_2} A_1} \quad (3)$$

so using (1) and (3) into (2) we get

$$A_1 = -\frac{k_1}{k_2} A_1 \tan k_2 a$$

$$\implies \frac{k_2}{k_1} = -\tan k_2 a$$

or $$\boxed{\sqrt{\frac{E}{V_0 - E}} = -\tan\left[\sqrt{\frac{2mE}{\hbar^2}}\, a\right]}$$ characteristic equation

- ~~If we plot LHS vs RHS~~ we will see that this equation is only valid for specific values of E

$\implies$ energy levels are quantized

- assume $V_0 = 2E \implies -1 = \tan\left[\underbrace{\sqrt{\frac{2mE}{\hbar^2}}\, a} + n\pi\right]$

periodic

$F = ma$ $\quad W = F \cdot d$

$\frac{kg \cdot m}{s^2}$

- For plotting, assum $a = 5\ \mathring{A}$

so $\rightarrow$ $-1 = \tan\left[\frac{\sqrt{2m}}{\hbar} a\sqrt{E} + n\pi\right]$

$$\frac{\sqrt{2m}}{\hbar} a = \frac{\sqrt{2(9.11\times10^{-31}\ kg)}}{1.054\times10^{-34}\ J\cdot s}(5\times10^{-10} m)$$

$$= 6.403\times10^{9}\ \frac{\sqrt{kg}}{kg\ \frac{m^{\cancel{2}}}{s^{\cancel{2}}}\cdot \cancel{s}}\cdot\cancel{m}$$

$$= 6.403\times10^{9}\ \frac{\sqrt{kg}}{kg\ \frac{m}{s}}$$

units are $\frac{\sqrt{kg}}{\cancel{\sqrt{kg}}\cdot\sqrt{kg}\ \frac{m}{s}} = \frac{1}{\sqrt{J}}$

so we have $6.403\times10^{9}\ \frac{1}{\sqrt{J}}$

convert to $\frac{1}{\sqrt{eV}}$: $6.403\times10^{9}\ \frac{1}{\cancel{\sqrt{J}}}\cdot\frac{(1.6\times10^{-19}\ \cancel{J})^{1/2}}{\sqrt{eV}}$

$$= 2.5612\ 1/\sqrt{eV}$$

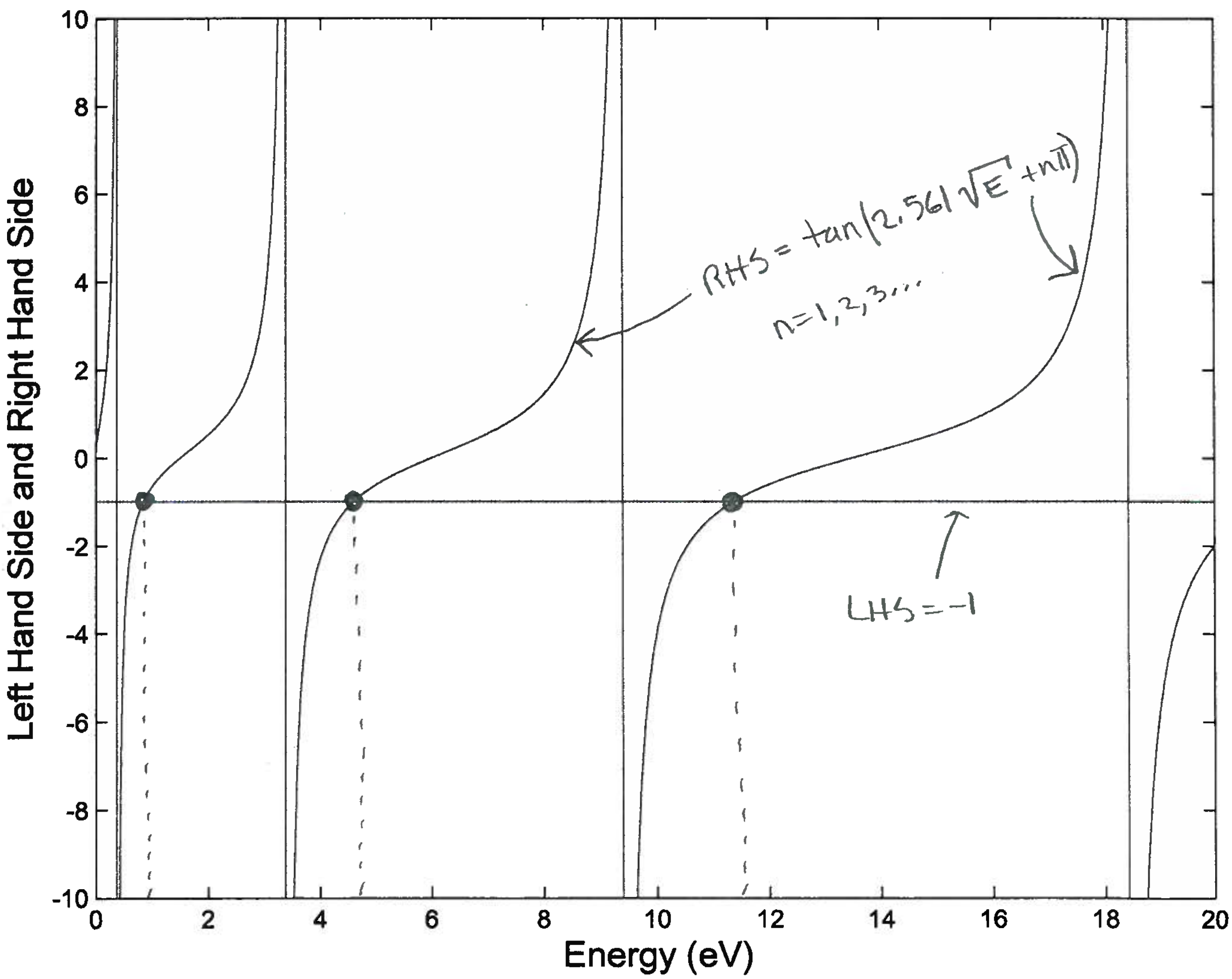
- so we have $-1 = \tan\left[2.5612\sqrt{E} + n\pi\right]$

where E is in [eV]

plot LHS & RHS (see attached plot)

$\hookrightarrow$ intersection points are the only allowed solutions for E

2.44



- dots show allowed values for E
- E is quantized

3.1

If the lattice constant (a_0) became smaller, the band gap would increase due to stronger interaction with the crystal.

If the lattice constant (a_0) became larger, the band gap would decrease

Larger bandgap $\Rightarrow$ behaves more like an isulator

Smaller bandgap $\Rightarrow$ behaves more like a metal

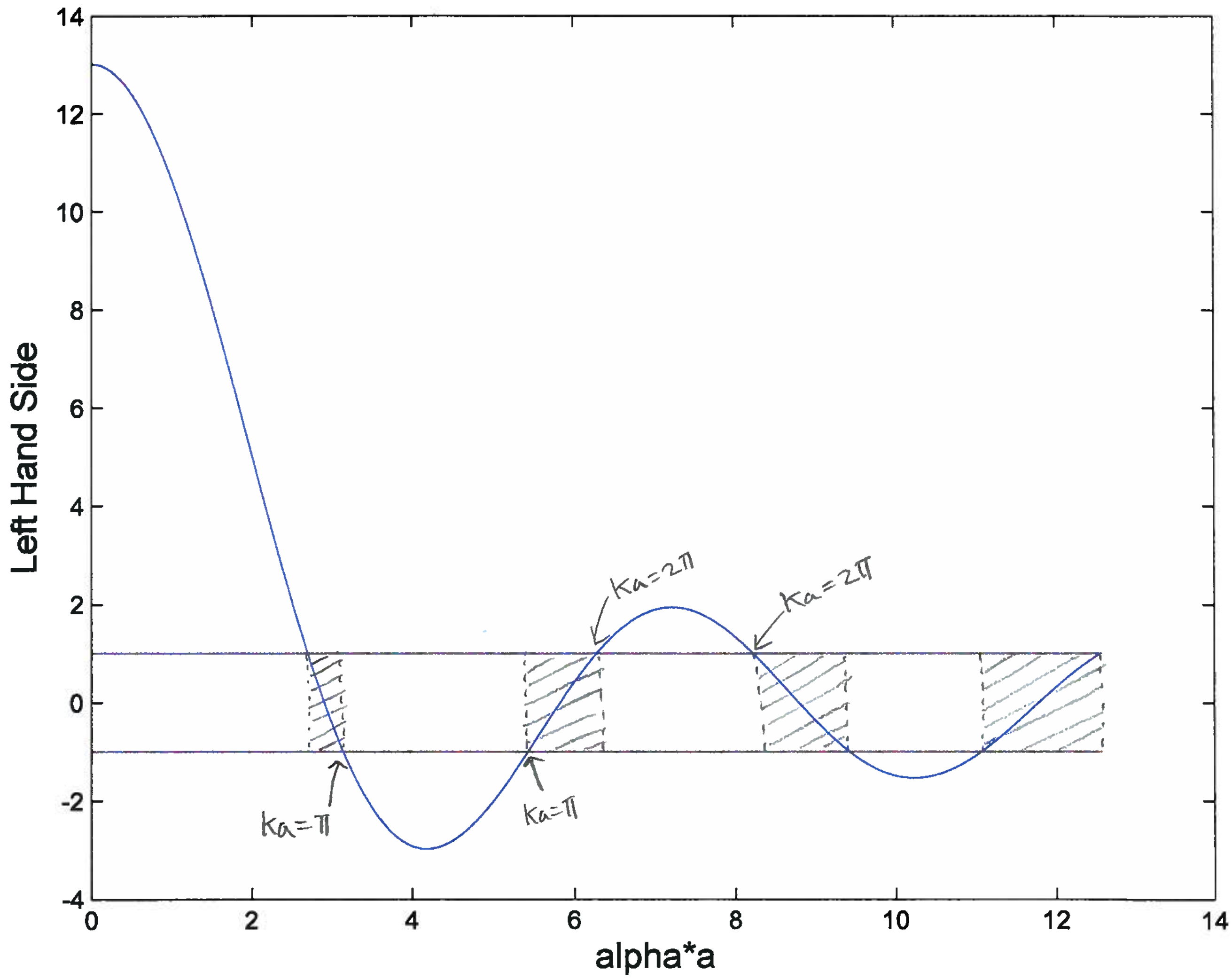
$\hookrightarrow$ when $E_g \to 0$

3.5 Plot $F(\alpha a) = \frac{12(\sin(\alpha a))}{\alpha a} + \cos(\alpha a)$ For $0 \le \alpha a \le 4\pi$

SEE Matlab plot

TOPS 35500

5.2



at $ka = \pi$: $\alpha a = \pi$, $\alpha a = 1.729\pi$

at $ka = 2\pi$: $\alpha a = 2\pi$, $\alpha a = 2.617\pi$

$\boxed{3.8}$ $a = 4.2$ Å , Free electron

- determine width of Forbidden bands that exist at
(a) $ka = \pi$ and (b) $ka = 2\pi$

(a) at $ka = \pi$ $\quad \alpha a = \pi$ and 1.729π

$$\alpha^2 = \frac{2mE}{\hbar^2} \Rightarrow E = \frac{\alpha^2 \hbar^2}{2m}$$

$$\alpha_1 = \frac{\pi}{a} = 7.48 \times 10^9 \ m^{-1}$$

$$\alpha_2 = \frac{1.729\pi}{a} = 1.29 \times 10^{10} \ m^{-1}$$

$$E_1 = \frac{(7.48 \times 10^9 m^{-1})^2 (1.054 \times 10^{-34} J \cdot s)^2}{2(9.11 \times 10^{-31} kg)}$$

$$= 3.41 \times 10^{-19} J = 2.132 \ eV$$

$$E_2 = \frac{(1.29 \times 10^{10} m^{-1})^2 (1.054 \times 10^{-34} J \cdot s)^2}{2(9.11 \times 10^{-31} kg)} = 1.015 \times 10^{-18} J$$

$$= 6.341 \ eV$$

so $E_{gap_\pi} = 6.341 - 2.132 \ eV \boxed{= 4.21 \ eV}$

b) at $ka = 2\pi$, $\alpha a = 2\pi$ and $\alpha a = 2.617\pi$

$$\alpha_1 = \frac{2\pi}{a} = 1.496 \times 10^{10} m^{-1}$$

$$\alpha_2 = \frac{2.617\pi}{a} = 1.96 \times 10^{10} \ m^{-1}$$

$$E_1 = \frac{(1.496 \times 10^{10} m^{-1})^2 (1.054 \times 10^{-34} J \cdot s)^2}{2(9.11 \times 10^{-31} kg)} = 1.365 \times 10^{-18} J$$

$$= 8.53 \ eV$$

$$E_2 = \frac{(1.96 \times 10^{10} m^{-1})^2 (1.054 \times 10^{-34} J \cdot s)^2}{2(9.11 \times 10^{-31} kg)} = 2.342 \times 10^{-18} J$$

$$= 14.64 \ eV$$

so $E_{gap_{2\pi}} = 14.64 - 8.53 \boxed{= 6.11 \ eV}$

3.9 $a = 4.2$ Å

determine the width in eV of the allowed energy bands for

(a) $0 < ka < \pi$

(b) $\pi < ka < 2\pi$

From 3.5, using the matlab plot

(a) at $ka = 0 \implies \alpha a = 2.699 \longrightarrow \alpha_1 = \frac{2.699}{a} = 6.43 \times 10^9$

at $ka = \pi \implies \alpha_2 a = \pi \implies \alpha_2 = \frac{\pi}{a} = 7.48 \times 10^9 m^{-1}$

so we get $\Delta E = \frac{\hbar^2}{2m}(\alpha_2^2 - \alpha_1^2)$

$$= \frac{(1.054 \times 10^{-34} J \cdot s)^2}{2(9.11 \times 10^{-31} kg)}\left[(7.48 \times 10^9 m^{-1})^2 - (6.43 \times 10^9 m^{-1})^2\right]$$

$$= 8.9 \times 10^{-20} J$$

$$\boxed{= 0.557 \text{ eV}}$$

(b) For the 2nd band

at $ka = \pi \implies \alpha a = 1.729\pi \implies \alpha_1 = \frac{1.729\pi}{a} = 1.29 \times 10^{10} m^{-1}$

at $ka = 2\pi \implies \alpha a = 6.283 \implies \alpha_2 = \frac{6.283}{a} = 1.50 \times 10^{10} m^{-1}$

$$\Delta E = \frac{(1.054 \times 10^{-34} J \cdot s)^2}{2(9.11 \times 10^{-31} kg)}\left[(1.50 \times 10^{10} m^{-1})^2 - (1.29 \times 10^{10} m^{-1})^2\right]$$

$$= 3.57 \times 10^{-19} J$$

$$\boxed{= 2.23 \text{ eV}}$$